

Excitation spectrum of the $S=1/2$ quantum spin ladder with frustration: elementary quasiparticles and many-particle bound states.

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Abstract

The excitation spectrum of the two-chain $S = 1/2$ Heisenberg spin ladder with additional second neighbor frustrating interactions is studied by a variety of techniques. A description, based on a mapping of the model onto a Bose gas of hard-core triplets is used to determine the one- and two-particle excitation spectra. We find that low-lying singlet and triplet bound states are present and their binding energy increases with increasing frustration. In addition, many-particle bound states are found by exact diagonalization and variational methods. We prove that the larger the number of bound particles the larger the binding energy. Thus the excitation spectrum has a complex structure and consists of elementary triplets and composite many-particle singlet and triplet bound states. The composite excitations mix strongly with the elementary ones in the coupling regime where quantum fluctuations are strong. The quantum phase transition, known to take place in this model at critical frustration is interpreted as a condensation process of (infinitely) large many-particle bound states.

I. INTRODUCTION

The $S = 1/2$ quantum spin ladder is relevant to a number of quasi one-dimensional compounds¹ and the list is growing as more materials become of experimental interest. Theoretically the two-leg ladder is, due to its geometry, the most simple realization of a "spin-liquid" - a quantum disordered state with gapped elementary excitations. The excitation spectrum of the ladder has been analyzed by a variety of techniques, including weak-coupling field theory mappings², exact diagonalization of small clusters^{3,4} and density-matrix renormalization group (DMRG) studies⁵. Also, strong-coupling techniques have been extensively used, such as dimer series expansions to high orders⁶ and mapping onto effective bosonic theories^{7,4,8}. The dispersion of the lowest triplet excitation as well as the gap in the spectrum are quite well understood within the aforementioned approaches.

Recently, an additional branch of excitations - two-magnon bound states were found in the spin ladder model^{9,8}. Such bound states were also predicted for the dimerized quantum spin chain¹⁰ which is another quantum system with a disordered ground state and gapped excitations. Bound states in quasi one-dimensional gapped spin systems have also been observed experimentally¹¹ although it is still not clear which one (or perhaps a combination of the two above¹²) is the relevant model for their description. Two of us have recently pointed out⁸ that bound states exist, in fact, in all one and two-dimensional quantum spin systems with dimerization of which the spin ladder and the dimerized chain are particular examples.

In the present paper we study the two-leg spin ladder with additional second neighbor frustrating interactions between the chains. This model was introduced quite recently and analyzed numerically via dimer series expansions¹³, DMRG¹⁴ and exact diagonalizations^{13,15}. A quantum phase transition was found as frustration increases from an antiferromagnetic (AF) ladder into Haldane (ferromagnetic ladder) phase. The excitation spectrum changes dramatically as one approaches the quantum transition point¹³. In a coupling region before the transition a singlet state appears in the triplet gap and at the transition both triplet and singlet gaps seem to approach zero^{13,15}. We will show in the present work that as frustration increases a number of low-energy many-particle bound states appear in the spectrum which mix strongly with the one-particle excitations. The energies of the bound states decrease with increasing frustration and number of particles forming them. Thus the quantum transition can be viewed as softening of a very complex excitation, composed of many-particle

bound states.

Consider the Hamiltonian of two coupled $S = 1/2$ chains (spin ladder):

$$H = \sum_i \left\{ J_{\perp} \mathbf{S}_i \cdot \mathbf{S}'_i + J \left(\mathbf{S}_i \cdot \mathbf{S}_{i+1} + \mathbf{S}'_i \cdot \mathbf{S}'_{i+1} \right) + J_2 \left(\mathbf{S}_i \cdot \mathbf{S}'_{i+1} + \mathbf{S}'_i \cdot \mathbf{S}_{i+1} \right) \right\}, \quad (1)$$

where the intra-chain (J) and the inter-chain (J_{\perp} , J_2) interactions are assumed antiferromagnetic $J, J_2, J_{\perp} > 0$. In Eq.(1) J_2 is a second neighbor inter chain coupling which causes frustration. In order to analyze the excitation spectrum of (1) it is convenient to adopt the strong-coupling viewpoint. At large $J_{\perp} \gg J, J_2$ the ground state consists of inter-chain spin singlets $|GS\rangle = |1, 0\rangle |2, 0\rangle |3, 0\rangle \dots$, where $|i, 0\rangle = \frac{1}{\sqrt{2}} [|\uparrow\rangle_i |\downarrow\rangle'_i - |\downarrow\rangle_i |\uparrow\rangle'_i]$. Since each singlet can be excited into a triplet state it is natural to introduce a creation operator $t_{\alpha i}^{\dagger}$ for this excitation:

$$|i, \alpha\rangle = t_{\alpha i}^{\dagger} |i, 0\rangle, \quad \alpha = x, y, z. \quad (2)$$

The representation of the spin operators in terms of $t_{\alpha i}^{\dagger}$ was introduced by Sachdev and Bhatt¹⁶:

$$S_{1,2}^{\alpha} = \frac{1}{2} (\pm t_{\alpha} \pm t_{\alpha}^{\dagger} - i \epsilon_{\alpha\beta\gamma} t_{\beta}^{\dagger} t_{\gamma}). \quad (3)$$

After application of this transformation to (1), or, equivalently, after calculating the matrix elements of the "hopping" terms J and J_2 in (1), we find:

$$H = \sum_{i, \alpha, \beta} \left\{ J_{\perp} t_{\alpha i}^{\dagger} t_{\alpha i} + \frac{\lambda}{2} \left(t_{\alpha i}^{\dagger} t_{\alpha i+1} + t_{\alpha i}^{\dagger} t_{\alpha i+1}^{\dagger} + \text{h.c.} \right) + \frac{\mu}{2} \left(t_{\alpha i}^{\dagger} t_{\beta i+1}^{\dagger} t_{\beta i} t_{\alpha i+1} - t_{\alpha i}^{\dagger} t_{\alpha i+1}^{\dagger} t_{\beta i} t_{\beta i+1} \right) \right\}, \quad (4)$$

where we have defined

$$\lambda = J - J_2, \quad \mu = J + J_2. \quad (5)$$

In addition, we have to restrict the Hilbert space by introducing the following hard-core on-site constraint¹⁶

$$t_{\alpha i}^{\dagger} t_{\beta i}^{\dagger} = 0. \quad (6)$$

This exclusion of double occupancy reflects the quantization of spin and ensures the uniqueness of the mapping from (1) to (4).

The Hamiltonian (1) as well as (4) is symmetric under permutation of the ladder legs. Therefore all excitations can be classified according to this symmetry. Following standard notations we will denote the antisymmetric excitations ($k_{\perp} = \pi$) by the index u and symmetric ones ($k_{\perp} = 0$) by the index g . It is clear that the operator $t_{\alpha i}$ (elementary triplet) corresponds to the u -excitation.

The rest of the paper is organized as follows. In Section II we describe the one-particle (triplet) excitation spectrum. In Section III the two-particle problem is considered and bound states in various channels are analyzed. Section IV addresses the bound state problem for many particles focusing mainly on the case of three particles. Section V presents our analysis of the quantum phase transition in light of the previous results and summarizes the work.

II. ELEMENTARY TRIPLET

At the quadratic level the Hamiltonian (4) can be diagonalized by a combination of Fourier and Bogoliubov transformations $t_{\alpha k} = u_k \tilde{t}_{\alpha k} + v_k \tilde{t}_{\alpha -k}^{\dagger}$. This gives the excitation spectrum: $\omega_k^2 = A_k^2 - B_k^2$, where $A_k = J_{\perp} + \lambda \cos k$ and $B_k = \lambda \cos k$. We find, in agreement with previous work^{16,7}, that the effect of the quartic terms in (4) on the triplet spectrum is small and therefore we proceed by treating these terms in mean field theory. This is equivalent to taking into account only one-loop diagrams (first order in μ). These diagrams lead to the renormalization:

$$A_k = J_{\perp} + (\lambda + 2\mu f_1) \cos k, \quad B_k = (\lambda - 2\mu g_1) \cos k, \quad (7)$$

where

$$\begin{aligned} f_1 &= \langle t_{\alpha i}^{\dagger} t_{\alpha i+1} \rangle = N^{-1} \sum_q v_q^2 \cos q \\ g_1 &= \langle t_{\alpha i} t_{\alpha i+1} \rangle = N^{-1} \sum_q u_q v_q \cos q. \end{aligned} \quad (8)$$

The above corrections are numerically quite small. The dominant contribution to the spectrum renormalization is related to the hard core condition Eq.(6). This condition is typically taken into account in the mean-field approximation^{7,16}. The latter is essentially uncontrolled, especially for a quasi-1D system. To deal with the constraint we will use the diagrammatic approach developed by us in Ref.[17]. An infinite on-site repulsion is introduced in this approach in order to forbid the double occupancy:

$$H_U = \frac{U}{2} \sum_{i,\alpha\beta} t_{\alpha i}^\dagger t_{\beta i}^\dagger t_{\beta i} t_{\alpha i}, \quad U \rightarrow \infty. \quad (9)$$

Since the interaction is infinite, the exact scattering amplitude $\Gamma_{\alpha\beta,\gamma\delta}(K) = \Gamma(K)(\delta_{\alpha\gamma}\delta_{\beta\delta} + \delta_{\alpha\delta}\delta_{\beta\gamma})$, $K \equiv (k, \omega)$, for the triplets has to be found. This quantity can be found by resumming the infinite series shown in Fig.1(a). One can easily see that Γ depends on the total energy and momentum of the incoming particles $K = K_1 + K_2$. The interaction (9) is local and non-retarded which allows us to obtain the analytic expression^{17,8} (in the limit $U \rightarrow \infty$)

$$\begin{aligned} \Gamma^{-1}(K) &= i \int \frac{d^2 Q}{(2\pi)^2} G(Q) G(K - Q) = \\ &= -\frac{1}{N} \sum_q \frac{u_q^2 u_{k-q}^2}{\omega - \omega_q - \omega_{k-q}} + \frac{1}{N} \sum_q \frac{v_q^2 v_{k-q}^2}{\omega + \omega_q + \omega_{k-q}}. \end{aligned} \quad (10)$$

Here $G(Q)$ is the normal Green's function (GF) $G(k, t) = -i\langle T(t_{k\alpha}(t)t_{k\alpha}^\dagger(0)) \rangle$:

$$G(k, \omega) = \frac{u_k^2}{\omega - \omega_k + i\delta} - \frac{v_k^2}{\omega + \omega_k - i\delta} \quad (11)$$

and the Bogoliubov coefficients $u_k^2, v_k^2 = \pm 1/2 + A_k/2\omega_k$. The basic approximation made in the derivation of $\Gamma(K)$ is the neglect of all anomalous scattering vertices, which are present in the theory due to the existence of anomalous GF's, $G_A(k, t) = -i\langle T(t_{-k\alpha}^\dagger(t)t_{k\alpha}^\dagger(0)) \rangle$.

$$G_A(k, \omega) = \frac{u_k v_k}{\omega - \omega_k + i\delta} - \frac{u_k v_k}{\omega + \omega_k - i\delta} \quad (12)$$

Our crucial observation¹⁷ is that all anomalous contributions are suppressed by a small parameter which is present in the theory - the density of triplet excitations $n_t = \sum_\alpha \langle t_{\alpha i}^\dagger t_{\alpha i} \rangle = 3N^{-1} \sum_q v_q^2$. We find that $n_t \approx 0.1$ ($J_\perp/J = 2$), $n_t \approx 0.25$ ($J_\perp/J = 1$) and it generally increases as J_\perp decreases. Since summation of ladders with anomalous GF's brings additional powers of v_q into Γ , their contribution is small compared to the dominant one of Eq.(10). In the following analysis we will take into account only the contributions to the self-energy which are at most linear in the triplet density n_t and therefore we also neglect the second term in Eq.(10). Thus our approach is expected to work as long as the gas of triplets is dilute enough (n_t is small).

The normal self-energy which includes only the first power of the amplitude Γ is given by the diagram in Fig.1(b):

$$\Sigma^{(Br)}(k, \omega) = \frac{4}{N} \sum_q v_q^2 \Gamma(k + q, \omega - \omega_q). \quad (13)$$

This is the dominant contribution to the spectrum renormalization as emphasized by Brueckner¹⁸ who developed the technique described above in order to study systems of strongly interacting fermions.

In the dilute gas approximation there are other diagrams which are formally at most linear in n_t but still numerically give contributions much smaller than the one of Eq.(13). The first one is the “rainbow” correction to the anomalous self-energy which is proportional to $\sqrt{n_t}$ and is shown in Fig.2(a):

$$\Sigma_A = \frac{1}{N} \sum_q u_q v_q \Gamma(0, 0). \quad (14)$$

This anomalous self-energy enforces the condition

$$\langle t_{\alpha i}^\dagger t_{\alpha i}^\dagger \rangle = N^{-1} \sum_k u_k v_k = 0. \quad (15)$$

The parameters u_k and v_k found in the zeroth approximation do not satisfy this condition. Taking into account the self energy (14) gives the corrected values of u_k and v_k which do satisfy (15). This can be seen from the formula for the renormalized Bogoliubov coefficients, Eq.(23) below. Since (14) is independent of k and ω , technically one can take into account the anomalous self-energy by introducing the term $\Lambda \sum_{i,\alpha} (t_{\alpha i}^\dagger t_{\alpha i}^\dagger + t_{\alpha i} t_{\alpha i})$ into the Hamiltonian (4) and choosing the Lagrange multiplier Λ from the condition (15).

The next correction is the contribution to the normal self-energy given by the diagram shown in Fig.2(b), where the square denotes the scattering amplitude (10). A standard calculation gives the expression for this diagram

$$\Sigma^{(2b)}(k, \omega) = \frac{6}{N^2} \sum_{p,q} \frac{(u_p v_p)(u_q v_q) u_{k+p-q}^2 \Gamma(k+p, \omega - \omega_p) \Gamma(k+q, \omega - \omega_q)}{\omega - \omega_p - \omega_q - \omega_{k+p-q}}. \quad (16)$$

Another correction is given by the diagram shown in Fig.2(c) plus the same diagram but with the positions of Γ and μ reversed. The result is

$$\Sigma^{(2c)}(k, \omega) = -\mu \frac{4}{N^2} \sum_{p,q} \frac{\cos(p-q)(u_p v_p)(u_q v_q) u_{k+p-q}^2 \Gamma(k+q, \omega - \omega_q)}{\omega - \omega_p - \omega_q - \omega_{k+p-q}}. \quad (17)$$

The last correction linear in the triplet density is shown at Fig.2(d). The corresponding expression is

$$\begin{aligned} \Sigma^{(2d)}(k, \omega) = & -\mu \frac{1}{N^3} \sum_{p,q,l} \frac{(u_p v_p)(u_q v_q) u_{k-p-l}^2 u_{k-q-l}^2 \Gamma(k-p, \omega - \omega_p) \Gamma(k-q, \omega - \omega_q)}{(\omega - \omega_p - \omega_l - \omega_{k-p-l})(\omega - \omega_q - \omega_l - \omega_{k-q-l})} \\ & \times [8 \cos(p+q+l-k) + 10 \cos(p-q)]. \end{aligned} \quad (18)$$

Let us stress again that all normal self-energy contributions (13),(16),(17),(18) are quadratic in v_q and hence linear in the triplet density. The anomalous self-energy (14) is linear in v_q and thus proportional to $\sqrt{n_t}$.

In order to find the renormalized spectrum, one has to solve the set of two coupled Dyson equations for the normal and anomalous GF's, shown symbolically in Fig.3. The result for the normal GF is:

$$G(K) = \frac{\omega + A_k + \Sigma(-K)}{[\omega + A_k + \Sigma(-K)][\omega - A_k - \Sigma(K)] + [B_k + \Sigma_A(K)]^2} \quad (19)$$

After separating this equation into a quasiparticle contribution and incoherent background, we find¹⁷:

$$G(k, \omega) = \frac{Z_k U_k^2}{\omega - \Omega_k + i\delta} - \frac{Z_k V_k^2}{\omega + \Omega_k - i\delta} + G_{inc}. \quad (20)$$

The renormalized triplet spectrum and the renormalization constant are:

$$\begin{aligned} \Omega_k &= Z_k \sqrt{[A_k + \Sigma(k, 0)]^2 - [B_k + \Sigma_A]^2}, \\ Z_k^{-1} &= 1 - \left(\frac{\partial \Sigma}{\partial \omega} \right)_{\omega=0}. \end{aligned} \quad (21)$$

Here the normal self-energy operator is given by Eqs.(13),(16),(17),(18)

$$\Sigma(k, \omega) = \Sigma^{(Br)} + \Sigma^{(2b)} + \Sigma^{(2c)} + \Sigma^{(2d)} \quad (22)$$

and the anomalous self-energy operator is given by Eq.(14). The renormalized Bogoliubov coefficients in (20) are:

$$U_k^2, V_k^2 = \pm \frac{1}{2} + \frac{Z_k [A_k + \Sigma(k, 0)]}{2\Omega_k}. \quad (23)$$

Equations (10,22, 21,23) have to be solved self-consistently for $\Sigma(k, 0)$ and Z_k . From Eq.(20) it also follows that one has to replace $u_k \rightarrow \sqrt{Z_k} U_k$, $v_k \rightarrow \sqrt{Z_k} V_k$ in all expressions presented above and below.

Let us demonstrate how this approach works in the strong-coupling limit $J_\perp \gg \mu, \lambda$. To first order in λ/J_\perp , $A_k = J_\perp + \lambda \cos k$ and $B_k = \lambda \cos k$. This leads to $\omega_k \approx A_k$, $u_k \approx 1$, $v_k \approx -(\lambda/2J_\perp) \cos k$ and $f_1 = 0$, $g_1 = -\lambda/4J_\perp$. Substitution into (10), (13), and (22) gives

$$\begin{aligned} \Gamma(k, \omega) &= 2J_\perp - \omega, \\ \Sigma(k, \omega) &= \Sigma^{(Br)}(k, \omega) = \frac{1}{2}(\lambda/J_\perp)^2(3J_\perp - \omega). \end{aligned} \quad (24)$$

Note that self-energy corrections (14), (16), (17), and (18) do not contribute in this order. Then from Eq.(21) we find the quasiparticle residue $Z = 1 - (1/2)(\lambda/J_\perp)^2$ and the dispersion

$$\Omega_k = J_\perp + \lambda \cos k + \frac{3\lambda^2}{4J_\perp} - \frac{\lambda^2}{4J_\perp} \cos 2k. \quad (25)$$

The result (25) agrees with that obtained by direct $1/J_\perp$ expansion¹⁹ to this order.

It is also useful to consider the next order in $1/J_\perp$. Using the first order calculation presented above we find $A_k = J_\perp + \lambda \cos k$ and $B_k = \lambda(1 + \mu/2J_\perp) \cos k$ and hence $u_k \approx 1$, $v_k \approx -B_k/2A_k \approx -(\lambda/2J_\perp)(1 + \mu/2J_\perp)(1 - \lambda/J_\perp \cos k) \cos k$. The scattering amplitude Γ is not changed in this order and thus given by Eq.(24). The anomalous self energy calculated according to Eq.(14) and the contributions to the normal self-energy given by Eqs.(13),(16), (17), (18) are:

$$\begin{aligned} \Sigma_A &= \lambda^2/2J_\perp(1 + \mu/2J_\perp), \\ \Sigma^{(Br)} &= \frac{1}{2}(\lambda/J_\perp)^2(1 + \mu/J_\perp)(3J_\perp - \omega), \\ \Sigma^{(2b)} &= \frac{3\lambda^3}{8J_\perp^2} \cos k, \\ \Sigma^{(2c)} &= \frac{\mu\lambda^2}{4J_\perp^2}, \\ \Sigma^{(2d)} &= -\frac{5\mu\lambda^2}{8J_\perp^2}. \end{aligned} \quad (26)$$

Substituting these into Eqs.(22),(21) we find the elementary triplet dispersion to order $1/J_\perp^2$:

$$\Omega_k = J_\perp + \lambda \cos k + \frac{\lambda^2}{J_\perp} \left(\frac{3}{4} - \frac{1}{4} \cos 2k \right) + \frac{\lambda^3}{J_\perp^2} \left(-\frac{1}{4} \cos k + \frac{1}{8} \cos 3k \right) + \frac{\lambda^2 \mu}{J_\perp^2} \left(\frac{3}{8} - \frac{1}{4} \cos 2k \right). \quad (27)$$

Using Eq.(23) one can also prove that the condition (15) is satisfied. The result (27) agrees with that obtained by direct $1/J_\perp$ expansion^{6,13} to this order.

The technique presented above is certainly not the simplest way to construct the $1/J_\perp$ expansion. Moreover it can not reproduce terms of order $1/J_\perp^3$ and higher because contributions to the self energies which are quadratic and higher order in the triplet density have been neglected in our approach. However the advantage of the method comes from the fact that n_t remains relatively small (0.25) even for $J/J_\perp = 1$. The purpose of the presented exercise was to demonstrate that the result of our approach coincides with the result obtained by perturbation theory around the dimer limit to the relevant order.

For arbitrary J_\perp a self-consistent numerical solution of Eqs.(10,13,21,23) is required. The triplet excitation spectra obtained from this solution for $J_\perp/J = 2$ are shown in Fig.4. For comparison we present the spectrum for $J_2 = 0$ which only includes the Brueckner correction (13) as well as the spectrum which includes all terms linear in n_t (the self-energies (14),(16),(17),(18), in addition to (13)). One can see that the Brueckner diagram is the most important one. All other corrections are much less important, however we will keep them in all subsequent calculations. Notice that the correlation corrections described above renormalize the spectrum very strongly as can be seen by comparing with the bare dispersion (all correlations neglected, $U = \mu = 0$): $\omega_k^2 = J_\perp^2 + 2\lambda J_\perp \cos k$. The bare spectrum even becomes unstable for $J_\perp < 2\lambda$. In Fig.4 we also present for comparison dispersions obtained by 8-th order dimer series expansion⁶. The agreement between our calculation and these curves is excellent which reflects the smallness of the triplet density $n_t \approx 0.1$. In Fig.5 we present similar plots for the case $J_\perp = J$. Looking at the curves at $J_2 = 0$ one can say that the agreement between our theory and the result obtained by series expansions is still reasonable because the triplet density in this case is $n_t \approx 0.25$ and hence one has to expect about 25% disagreement. However as J_2 increases the disagreement increases (especially at the point $k = 0$) in spite of the fact that according to our calculation the triplet density does not increase and even slightly decreases. Moreover the excitation energy at $k = 0$ vanishes at $J_2 \approx 0.6J$, which signals a quantum phase transition into the Haldane phase. Our calculation however does not give any indication of the triplet mode becoming soft at $k = 0$. Therefore something important is missing in our approach. We will demonstrate in Section IV that what is missing is the contribution of low-energy many-particle bound states (3,5,7... particles) which have u -symmetry and therefore can mix with the elementary triplet.

Next, we proceed with the analysis of two-particle bound states which have g -symmetry and therefore do not mix with the elementary triplet.

III. TWO-PARTICLE BOUND STATES

The quartic interaction in the Hamiltonian (4) leads to attraction between two triplet excitations. We will show that the attraction is strong enough to form a singlet ($S=0$) and a triplet ($S=1$) bound state. The method we employ essentially follows our previous work⁸.

Consider the scattering of two triplets: $q_1\alpha + q_2\beta \rightarrow q_3\gamma + q_4\delta$ and introduce the total

(Q) and relative (q) momentum of the pair $q_1 = Q/2 + q$, $q_2 = Q/2 - q$, $q_3 = Q/2 + p$, and $q_4 = Q/2 - p$. The bare (Born) scattering amplitude is (see Fig.6(a)):

$$\begin{aligned} M_{\alpha\beta,\gamma\delta} = & \mu (\delta_{\alpha\gamma}\delta_{\beta\delta} - \delta_{\alpha\beta}\delta_{\gamma\delta}) \cos(q + p) + \\ & \mu (\delta_{\alpha\delta}\delta_{\beta\gamma} - \delta_{\alpha\beta}\delta_{\gamma\delta}) \cos(q - p) + \\ & U(\delta_{\alpha\gamma}\delta_{\beta\delta} + \delta_{\alpha\delta}\delta_{\beta\gamma}). \end{aligned} \quad (28)$$

The μ and the U terms arise from the quartic interaction in (4) and the constraint (9) respectively. We also have to take into account that the triplet excitation differs from the bare one due to the Bogoliubov transformation and the quasiparticle residue. Therefore the following substitution has to be made:

$$M_{\alpha\beta,\gamma\delta} \rightarrow \sqrt{Z_{q_1}} U_{q_1} \sqrt{Z_{q_2}} U_{q_2} \sqrt{Z_{q_3}} U_{q_3} \sqrt{Z_{q_4}} U_{q_4} M_{\alpha\beta,\gamma\delta}. \quad (29)$$

The bound state satisfies the Bethe-Salpeter equation for the poles of the exact scattering amplitude \tilde{M} . This equation is presented graphically in Fig.6(b) and has the form²⁰:

$$\left[E_Q - \Omega_{Q/2+q} - \Omega_{Q/2-q} \right] \psi(q) = \frac{1}{2} \int \frac{dp}{2\pi} M(Q, q, p) \psi(p). \quad (30)$$

Here $M(Q, q, p)$ is the scattering amplitude in the appropriate channel, E_Q is the energy of the bound state and $\psi(q)$ is the two-particle wave function. The factor of 2 in Eq.(30) is related to the symmetry of the diagram on the right hand side of Fig.6(b) under the exchange of the two intermediate lines. Thus in order to avoid double counting of the intermediate states, the result has to be divided by two. Let us introduce the minimum energy for two excitations with given total momentum (lower edge of the two-particle continuum) $E_Q^c = \min_q \{ \Omega_{Q/2+q} + \Omega_{Q/2-q} \}$. If a bound state exists then its energy is lower than the continuum $E_Q < E_Q^c$. The binding energy is defined as $\epsilon_Q = E_Q^c - E_Q > 0$.

In the singlet ($S=0$) channel the scattering amplitude is:

$$M^{(0)} = \frac{1}{3} \delta_{\alpha\beta} \delta_{\gamma\delta} M_{\alpha\beta,\gamma\delta} = -4\mu \cos q \cos p + 2U. \quad (31)$$

First, consider the strong-coupling limit $J_\perp \gg J, J_2$. Let us keep terms up to first order in $1/J_\perp$, i.e. take Ω_q from Eq.(25). The lower edge of the continuum in this order is:

$$E_Q^c = 2J_\perp + \frac{3\lambda^2}{2J_\perp} + \begin{cases} -\frac{\lambda^2}{2J_\perp} \cos Q - 2\lambda \cos Q/2 & , Q < Q^* \\ +\frac{\lambda^2}{2J_\perp} \cos Q + J_\perp (\cos^2 Q/2) / \cos Q & , Q > Q^* \end{cases} \quad (32)$$

Here Q^* is determined from the equation: $(\cos Q^*/2)/\cos Q^* = -\lambda/J_\perp$. Notice that in the strict limit $\lambda/J_\perp = 0$ one has $Q^* = \pi$ and thus the upper line in Eq.(32) is sufficient. The equation for the bound state reads:

$$\left[E_Q^{(0)} - 2J_\perp - 2\lambda \cos Q/2 \cos q - \frac{3\lambda^2}{2J_\perp} + \frac{\lambda^2}{2J_\perp} \cos Q \cos 2q \right] \psi(q) = -2\mu \cos q \int \frac{dp}{2\pi} \cos p \psi(p) + U \int \frac{dp}{2\pi} \psi(p). \quad (33)$$

Since we work to order $1/J_\perp$ and both $Z_q, U_q = 1 + O(\lambda^2/J_\perp^2)$, these quantities have been set to unity in (33). Due to the infinite repulsion ($U \rightarrow \infty$), a Lagrange multiplier has to be introduced to enforce the condition $\int dp \psi(p) = 0$ (meaning that the bound state is d-wave like). The solution of Eq.(33) to leading order for the wave-function and next to leading order for the energy is:

$$\psi^{(0)}(q, Q) = \sqrt{2(1 - C_Q^2)} \frac{\cos q + C_Q}{1 + C_Q^2 + 2C_Q \cos q} + O\left(\frac{\lambda^2}{\mu J_\perp}\right) \quad (34)$$

$$E_Q^{(0)} = 2J_\perp + \frac{3\lambda^2}{2J_\perp} - \mu(1 + C_Q^2) - \frac{\lambda^2}{4J_\perp}(1 + C_Q^2) \cos Q \quad (35)$$

where we have introduced the notation

$$C_Q = \frac{\lambda}{\mu} \cos Q/2. \quad (36)$$

Thus we see that in the strong-coupling limit a singlet bound state always exists. At $J_\perp = 2J$, $J_2 = 0$ Eq.(30) with the substitution (29) has to be solved numerically and the result is presented in Fig.7. We find that for $k \lesssim 2\pi/5$ the binding energy is practically zero in this case.

In the triplet (S=1) channel the scattering amplitude is:

$$M^{(1)} = \frac{1}{2} \epsilon_{\rho\alpha\beta} \epsilon_{\rho\gamma\delta} M_{\alpha\beta, \gamma\delta} = -2\mu \sin q \sin p. \quad (37)$$

In this formula there is no summation over the index ρ which gives the spin of the bound state. By solving Eq.(30) in the limit $J_\perp \gg J, J_2$ we obtain for the wave-function and the binding energy:

$$\psi^{(1)}(q, Q) = \sqrt{1/2 - 2C_Q^2} \frac{\sin q}{1/2 + 2C_Q^2 + 2C_Q \cos q} + O\left(\frac{\lambda^2}{\mu J_\perp}\right) \quad (38)$$

$$E_Q^{(1)} = 2J_\perp + \frac{3\lambda^2}{2J_\perp} - \frac{\mu}{2}(1 + 4C_Q^2) - \frac{\lambda^2}{2J_\perp}(6C_Q^2 - 1/2) \cos Q, \quad C_Q < 1/2. \quad (39)$$

For $C_Q > 1/2$ we find that the binding energy vanishes, $\epsilon_Q^{(1)} = E_Q^c - E_Q^{(1)} = 0$, which means that at $J_2 = 0$ ($\mu = \lambda = J$) the triplet bound state only exists for momenta $k > Q_c = 2\pi/3$ (in the strong-coupling limit)⁹. At $J_\perp = 2J$, $J_2 = 0$ the numerical solution of Eq.(30), plotted in Fig.7 (with the additional contribution Eq.(41)) shows that the bound state exists down to $k \approx \pi/2$.

Finally, we find that there is no bound state in the tensor (S=2) channel. This is due to the fact that the scattering amplitude in this case $M^{(2)} = 2\mu \cos q \cos p + 2U$ corresponds to repulsion and consequently there is no solution of the Bethe-Salpeter equation with positive binding energy. However a solution exists with energy above the upper edge of the two-particle continuum. In the simplest case $J = J_2, \lambda = 0$ we find to leading order $E^{(2)} = 2J_\perp + \mu/2$ and thus the "anti-binding" energy is $\mu/2$.

Equation (30) takes into account the potential interaction between two dressed elementary triplets, but it does not take into account the contribution of quantum fluctuations into binding. Let us consider this effect. In the strong coupling limit the first correction to the ground state energy of the system is due to the term $\frac{\lambda}{2} t_{\alpha i}^\dagger t_{\alpha i+1}^\dagger$ in the Hamiltonian (4) which virtually excites a pair of triplets. Thus the energy correction per link to lowest order is

$$\delta E_0 = -3 \frac{(\lambda/2)^2}{2J_\perp}, \quad (40)$$

where the coefficient 3 is due to the number of possible polarizations²¹. When we have a state with a real elementary triplet, the quasiparticle (triplet) blocks virtual excitations on two links and this increases its energy by $2|\delta E_0|$. This is the physical origin of the third term in the dispersion (25). Now let us consider two quasiparticles. When they are separated by more than one lattice spacing they block four links, but when they are on nearest neighbor sites they block only three links. This gives an effective attraction δE_0 . However two quasiparticles in a singlet (S=0) state can virtually annihilate because of the term $\frac{\lambda}{2} t_{\alpha i} t_{\alpha i+1}$ in the Hamiltonian (4) which has the same tensor structure. This term gives $-\delta E_0$ and consequently the net effective attraction due to quantum fluctuations vanishes. For the triplet (S=1) bound state there is no annihilation and therefore the energy level shift due to blocking of quantum fluctuations is²²

$$\delta E_Q^{(1)} = \delta E_0 \left| \int \sqrt{2} \sin q \psi^{(1)}(q, Q) \frac{dq}{2\pi} \right|^2. \quad (41)$$

The integral gives the probability amplitude for two quasiparticles to be on nearest neighbor sites. The two-particle triplet (S=1) bound state energy for $J_\perp = 2J$, $J_2 = 0$ is plotted in

Fig.7 where the potential contribution as well as Eq.(41) have been taken into account. While in the strong coupling limit the binding in the triplet channel is weaker than the one in the singlet channel (as can be seen from Eqs.(35),(39)), for $J_\perp = 2J$, $J_2 = 0$ the additional attraction due to blocking of quantum fluctuations pushes the triplet below the singlet for the range of momenta $4\pi/5 \lesssim q < \pi$.

The sizes of the bound states can be determined from the corresponding wave functions. As expected the size increases with decreasing binding energy and near the threshold we find $R_{rms} \sim (\epsilon)^{-1/2}$, $\epsilon \rightarrow 0$. The self-consistent evaluation of the sizes shows that both bound states typically extend over a few lattice spacings⁸.

The quantity which is directly measurable in inelastic neutron scattering experiments is the dynamical structure factor:

$$S_{g,u}(k, \omega) = \int e^{i\omega t} \langle S_z^{g,u}(k, t) S_z^{g,u}(-k, 0) \rangle dt, \quad S_{z,i}^{g,u} = S_{z,i} \pm S'_{z,i} \quad (42)$$

The superscript corresponds to transverse (along the rungs) momentum $k_\perp = 0, \pi$, i.e. $S_{z,i}^{g,u} = S_{z,i} \pm S'_{z,i}$. The symmetric combination ($k_\perp = 0$) gives the magnetic moment of the elementary triplet which is equal to unity. Therefore expressed in terms of Cartesian components the magnetic moment has the form $M_\mu = -i\epsilon_{\mu\alpha\beta} t_\alpha^\dagger t_\beta$. This immediately gives

$$S_{z,i} + S'_{z,i} = -i\epsilon_{z\alpha\beta} t_{\alpha i}^\dagger t_{\beta i} \rightarrow -i\epsilon_{z\alpha\beta} \sum_q u_q v_{k-q} \tilde{t}_{\alpha q}^\dagger \tilde{t}_{\beta k-q}^\dagger, \quad (43)$$

where we also have taken into account the Bogoliubov transformation. By projecting this operator onto the bound state wave function we find the contribution of the $S = 1$ bound state to the static structure factor $S_g(k) = \int S_g(k, \omega) d\omega / 2\pi$:

$$S_g(k) = 4 \left[\frac{1}{N} \sum_q \psi^{(1)}(q, k) u_{k/2+q} v_{k/2-q} \right]^2 = \frac{1}{2} (\lambda/J_\perp)^2 \sin^2 k / 2 (1 - 4C_k^2) + O(\lambda^4/J_\perp^4). \quad (44)$$

In this formula C_k is defined by Eq.(36). The substitution $(u_k, v_k) \rightarrow \sqrt{Z_k}(U_k, V_k)$ has to be made according to (20) in order to find the result for arbitrary J_\perp/J . We have also presented the leading order of the strong coupling expansion.

A similar calculation in the u channel, i.e. for the elementary triplet gives

$$S_u(k) = (u_k + v_k)^2 = 1 - \frac{\lambda}{J_\perp} \cos k + O(\lambda^2/J_\perp^2). \quad (45)$$

For $J_2 = 0$, $J_\perp = 2J$ we have found by numerical evaluation of the corresponding expressions that $S_g(\pi)/S_u(\pi) \approx 0.05$ and thus the experimental signal is expected to be about 20 times weaker for the bound state compared to the elementary triplet⁸.

IV. MANY-PARTICLE BOUND STATES

Let us first consider a three-particle bound state with total spin $S=1$ (triplet). This state consists of an odd number of elementary triplets and hence has u -symmetry. A convenient way to solve the three-particle problem is to use the variational method. First consider the simplest ansatz: three triplet excitations on nearest neighbor sites. Such ansatz is valid in the limit of zero hopping ($\lambda = 0$). A straightforward minimization of the expectation value of the Hamiltonian (4) gives the energy and the wave function of this state:

$$|k\rangle_\rho = \frac{1}{\sqrt{8}} (\delta_{\alpha\rho}\delta_{\beta\gamma} + \delta_{\gamma\rho}\delta_{\alpha\beta}) \sum_n e^{ikn} t_{\alpha,n-1}^\dagger t_{\beta,n}^\dagger t_{\gamma,n+1}^\dagger |0\rangle, \quad (46)$$

$${}_\rho\langle k|H|k\rangle_\rho = 3J_\perp - 1.25\mu,$$

where k and ρ are the momentum and the polarization of the state. Next, one can extend this ansatz by allowing each triplet to hop onto a nearby site (first order in λ):

$$\psi_\rho(k) = a|k\rangle_\rho + b|k\rangle'_\rho, \quad (47)$$

$$|k\rangle'_\rho = \frac{1}{\sqrt{16}} (\delta_{\alpha\rho}\delta_{\beta\gamma} + \delta_{\gamma\rho}\delta_{\alpha\beta}) \sum_n e^{ikn} (t_{\alpha,n-2}^\dagger t_{\beta,n}^\dagger t_{\gamma,n+1}^\dagger + t_{\alpha,n-2}^\dagger t_{\beta,n}^\dagger t_{\gamma,n+2}^\dagger) |0\rangle.$$

The state $\psi_\rho(k)$ must also be normalized, i.e. $a^2 + b^2 = 1$. The Hamiltonian has to be calculated in this basis, and additionally the energy level shifts due to blocking of quantum fluctuations have to be included, similarly to the discussion in the previous section. The result for the effective Hamilton matrix is:

$$\langle H \rangle_{eff} = \begin{pmatrix} 3J_\perp - 1.25\mu + 2\frac{\lambda^2}{J_\perp} & \frac{\lambda}{\sqrt{2}} \\ \frac{\lambda}{\sqrt{2}} & 3J_\perp - \mu + \frac{\lambda}{2} \cos k + \frac{17}{8} \frac{\lambda^2}{J_\perp} \end{pmatrix} \quad (48)$$

Notice that the quantum fluctuation correction in the second diagonal term ($\frac{17}{8} \frac{\lambda^2}{J_\perp}$) is slightly larger than the one in the first term. This is the same effect as the one discussed in the previous section - effective attraction due to suppression of quantum fluctuations. In this situation numerically this attraction is not very important. The energy of the three-particle bound state is

$$E_3(k) = 3J_\perp - \frac{9}{8}\mu + \frac{\lambda}{4} \cos k + \frac{33}{16} \frac{\lambda^2}{J_\perp} - \sqrt{\left(\frac{\mu}{8} + \frac{\lambda}{4} \cos k + \frac{1}{16} \frac{\lambda^2}{J_\perp}\right)^2 + \frac{\lambda^2}{2}}. \quad (49)$$

Consider first the strong coupling limit, $J_\perp \gg J, J_2$. For $J_2 = 0$ (i.e. $\mu = \lambda = J$) eq. (49) gives

$$\begin{aligned}
E_3(k=0) &= 3J_\perp - 1.68J, \\
E_3(k=\pi) &= 3J_\perp - 2.09J.
\end{aligned}
\tag{50}$$

The state with $k = \pi$ is unstable with respect to decay into three elementary triplets because the energy of the elementary triplet is $\Omega_q = J_\perp + J \cos q$. However the state with $k = 0$ is stable with respect to this decay. Nevertheless this state is also unstable since it can decay into a two-triplet bound state (Section III) and an elementary triplet. The threshold for this decay is $3J_\perp - 2J$ which is pretty close to $E_3(0)$ given by (50). Therefore a quite natural question arises: can improvements of the variational wave function push the energy $E_3(0)$ below the threshold? To check this we extended the ansatz (47) by including states with double hopping (order λ^2): $t_{n-3}^\dagger t_n^\dagger t_{n+1}^\dagger$, $t_{n-1}^\dagger t_n^\dagger t_{n+3}^\dagger$, and $t_{n-2}^\dagger t_n^\dagger t_{n+2}^\dagger$. We find that $E_3(0)$ decreases to the value $3J_\perp - 1.77J$, but still remains above the decay threshold. Therefore we believe that in the strong coupling limit for $J_2 = 0$ the three-particle bound state does not exist. However when $J_2 > (0.3 - 0.4)J$ the bound state at $k = 0$ becomes stable which follows immediately from Eq.(49).

For intermediate values of J_\perp the three-particle state becomes stable for any J_2 . Let us consider three cases for $J_\perp = 2J$. According to Eq.(49)

$$\begin{aligned}
J_2 = 0 : \quad & E_3(k=0) = 5.3J, \quad E_3(k=\pi) = 4.9J, \\
J_2 = 0.4J : \quad & E_3(k=0) = 4.4J, \quad E_3(k=\pi) = 4.2J, \\
J_2 = 0.8J : \quad & E_3(k=0) = 3.7J, \quad E_3(k=\pi) = 3.7J.
\end{aligned}
\tag{51}$$

In all these cases any decay of the $k = 0$ state is kinematically forbidden (this can be found from comparison with the elementary triplet and two-particle bound state spectra presented in Figs.4,7).

Next, we compare the variational results with numerical exact diagonalization results we have obtained for a 2×10 ladder. Plots of the spectral function $A(k, \omega) = -\pi^{-1} \text{Im} G(k, \omega + i\delta)$ in the u -channel (odd number of particles) for $k = 0$ found by Lanczos diagonalization of the Hamiltonian (1) are presented in Fig.8. The first peak corresponds to the elementary triplet and the second one to the three-particle bound state. The positions of the second peak agree very well with Eq.(51). For $k = \pi$ we find numerically that a second peak is absent for $J_2 = 0, 0.4J$ whereas a peak with an extremely small spectral weight seems to exist for $J_2 = 0.8J$. This can be understood from the variational treatment since the state $k = \pi$ can decay into three elementary triplets (compare (51) and

Fig.4) for $J_2 = 0$. Even though this state is slightly below the threshold for $J_2 = 0.4J$, due to the limited accuracy of our calculation it is really hard to say whether it decays or not. However for $J_2 = 0.8J$ the state $k = \pi$ is well below the decay threshold, and indeed a peak exists in the corresponding spectral function. Thus we believe that the variational method captures quite accurately the main features of the spectrum.

For $J_\perp = J$ according to Eq.(49) the three-particle bound state energy is

$$\begin{aligned} J_2 = 0 : \quad E_3(k=0) &= 3.3J, \quad E_3(k=\pi) = 3.0J, \\ J_2 = 0.4J : \quad E_3(k=0) &= 1.8J, \quad E_3(k=\pi) = 1.6J, \\ J_2 = 0.6J : \quad E_3(k=0) &= 1.2J, \quad E_3(k=\pi) = 1.1J, \end{aligned} \tag{52}$$

Comparing with the exact diagonalization spectra presented in Fig.9 and Fig.10 one can see that the overall agreement is good. Notice that while for $J_2 = 0$ the variational energies are higher than the numerical ones (as one would expect), for $J_2 = 0.4J, 0.6J$ they are in fact lower. We attribute this effect to the mixing between the three-particle and the elementary triplet which has not been taken into account in our approach (see the discussion below).

In the numerical spectra in Fig.9 and Fig.10 a third peak is also clearly seen. This is the five-particle bound state. To estimate its energy as well as the energies of bound states containing higher number of particles we could use the $N = \infty$ approximation (N is the number of particles). In the limit $\lambda = 0$ the quartic term in the Hamiltonian Eq.(4) is identical to the Hamiltonian of an $S = 1$ Heisenberg chain with antiferromagnetic interaction $\mu/2$. The ground state energy of the latter (for an infinite chain) is known quite accurately to be -0.700742μ per link²³. Therefore a crude estimate for the energy of an N -particle bound state (containing $N - 1$ links) is

$$E_N = NJ_\perp - (N - 1) \times 0.7\mu, \tag{53}$$

For the five-particle bound state by using the above formula and taking also into account the increase in energy due to blocking of quantum fluctuations ($3\lambda^2/J_\perp$), we obtain $E_5 \approx 4.5J$ for $J_\perp = J$, $J_2 = 0$, and $E_5 \approx 1.9J$ for $J_\perp = J$, $J_2 = 0.4J$, in qualitative agreement with the numerical results presented in Figs.9,10.

Now we can address the problem formulated at the end of Sec.II: Why the diagrammatic approach developed in Sec.II, which works quite well for $J_2 = 0$, does not describe even qualitatively the triplet energy spectrum for $J_\perp = J$ and $J_2 > 0$?. In light of the results of the present section, we find that the essence of the problem is in the neglect of bound

states of three, five, etc. quasiparticles whose energies decrease with increasing J_2 . Indeed, let us fix $J_2 = 0.4J$ and compare the energy of the elementary triplet at zero momentum from Fig.5 (dashed line), $\Omega_0 \approx 1.73J$, with the energies of the three- and five-particle bound states $E_3(k=0) \approx 1.8J$, $E_5(k=0) \approx 1.9J$. They are quite close, and since all these states have the same quantum numbers they mix strongly. Notice that in the calculation of the one-particle properties as well as the three-particle problem we have not taken the mixing into account. Thus we expect the wave function in the u -sector (and similarly for the g -sector) to be a superposition of states with different numbers of quasiparticles:

$$|\Psi\rangle = Z_1|\Psi\rangle^{(1)} + Z_3|\Psi\rangle^{(3)} + Z_5|\Psi\rangle^{(5)} + \dots \quad (54)$$

In this situation the classification of the states by the number of "elementary" quasi particles is becoming meaningless, and the average number of excited triplets in the lowest excitation at $k=0$ is increasing. The full description of the energy spectrum requires the determination of the mixing coefficients in Eq.(54) which is beyond the scope of the present work and will be reported in the future. We expect that the energy of the "elementary" triplet will lower substantially at $k=0$ (with respect to the "naive" calculation of Sec.II) due to repulsion from the nearby many-particle bound states. In addition, as can be seen from the analysis of the three- and five-particle bound states, the larger J_2 the larger the number of many-particle bound states which have low energies and mix with the "elementary" triplet. In fact it becomes energetically more and more favorable to form states with larger and larger number of quasiparticles in them as J_2 increases. Thus we expect that the quasiparticle residue will decrease with increasing J_2 - an effect which indeed can be seen from our numerical analysis (see Fig.9 for $J_2 = 0.6J$). Eventually a situation may occur when the quasiparticle residue has vanished completely which means that very large size bound states completely dominate in the wave function Eq.(54). This is the point where there is an excited triplet on every site and the ground state changes its nature.

V. QUANTUM PHASE TRANSITION IN THE MODEL. SUMMARY AND CONCLUSIONS.

The analysis of the previous section allows us to shed new light onto the nature of the quantum phase transition which takes place in the frustrated ladder model. The phase diagram of the model was determined in Ref.[13] and is presented in Fig.11. At a critical

coupling $J_{2c}(J_{\perp})$ the ground state changes from that of an antiferromagnetic (AF) spin ladder to a ladder with an effective ferromagnetic interaction on the rungs (Haldane phase). From the point of view of the triplet excitations in the AF ladder phase, the Haldane phase is characterized by an excited triplet on every rung. Thus it is not surprising that bound states of many-particles become favorable energetically near the quantum transition point.

The analysis of the energy spectrum is particularly simple on the line $J_2 = J(\lambda = 0)$ where quantum fluctuations are absent completely. It is known that on this line there is an exact eigenstate of the Hamiltonian (4) which is a product of singlets (dimers) on each rung²⁴. This is obvious from Eq.(4). This state is the ground state in the region $J_{\perp} > 1.4J$ (see below). As J_{\perp} decreases from a large value and approaches the quantum critical point, a number of singlet states appear in the triplet gap. Figure 12 presents a plot of the elementary triplet ($u1$), two-particle singlet ($g2$), three-particle triplet ($u3$) and four-particle singlet ($g4$). The energies of these states have been found by analytical diagonalization of the Hamiltonian Eq.(4): $E_{u1} = J_{\perp}$, $E_{g2} = 2J_{\perp} - 2J$, $E_{u3} = 3J_{\perp} - 2.5J$, $E_{g4} = 4J_{\perp} - 4.46J$. It is clear that at the point $J_2 = 2J$ the two-particle singlet crosses the one-particle triplet and thus becomes the lowest excitation in the system. Also we observe that the larger the number of bound particles the larger the rate of decrease of their energy. For comparison we have also schematically plotted the states $u9$ and $g10$. Thus we see that a number of singlets appear in the triplet gap and many level crossings take place. Notice that there is no mixing between the states since quantum fluctuations are absent ($\lambda = 0$). At the point $J_{\perp,c} = 1.4J$ the energy of the singlet composed of infinitely many quasiparticles becomes zero, $E_{g\infty} = 0$, as can be seen from Eq.(53). The triplet (u) bound state energies do not cross the elementary triplet for any finite number of particles in them, however the infinite particle triplet becomes degenerate with the corresponding singlet $E_{u\infty} = E_{g\infty} = 0$ at the transition point (this also follows from Eq.(53)).

We believe that the picture of the quantum transition presented above remains valid along the whole critical line (Fig.11). The transition is characterized by softening of the singlet and triplet (at $k = 0$) modes which are basically very large size bound states of many quasiparticles in the appropriate channel. Slightly away from the critical line (on the AF side) the excitation wave function is a mixture of bound states with different number of particles and the weight of the large-size bound states increases as the transition is approached.

In summary, we have analyzed the properties of many-particle bound states in the frus-

trated ladder model. We have found that the excitation spectrum is quite complex and many-particle bound states are always present in the model. Frustration pushes the bound states to lower energies and the effective triplet and singlet spectra are very strongly renormalized with respect to the simple ladder (no frustration). Thus the model is an ideal playground for studying complex excitations in quantum spin systems.

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²⁰ Equation (30) can also be derived as a two-particle Schrödinger equation in momentum space $H\Psi_Q = E_Q\Psi_Q$. For the singlet bound state one has $\Psi_Q = \sum_q \psi^{(0)}(q, Q) t_{\alpha, q_1}^\dagger t_{\alpha, q_2}^\dagger |0\rangle$, where $q_{1,2}$ are defined in the text before Eq.(28). For a triplet bound state with polarization α : $\Psi_{Q,\alpha} = \sum_q \psi^{(1)}(q, Q) \epsilon_{\alpha\beta\gamma} t_{\beta, q_1}^\dagger t_{\gamma, q_2}^\dagger |0\rangle$. While this way of deriving the Bethe-Salpeter equation is quite simple and physically transparent, the approach presented in the text is more general and we give it preference since it is better suited for treating more complicated interaction terms (e.g. three-body interactions which appear in certain models with dimerization¹⁷).

²¹ Strictly speaking Eq.(40) is valid for $J_\perp \gg J, J_2$. However it works quite well even for $J_\perp \sim J$. For example at the point $J_\perp = J, J_2 = 0$, according to Eq.(40) $\delta E_0 = -0.375J$ while the numerical result^{6,13} is $\delta E_0 = -0.406J$.

²² This effect is similar to the shift of energy levels due to radiative corrections in relativistic atomic physics (Lamb shift).

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FIGURES

FIG. 1. (a) Resummation of the infinite ladder for the scattering amplitude Γ . The dashed line represents the (infinite) two-particle interaction U . (b) The self-energy, corresponding to Γ .

FIG. 2. Diagrams for the self-energy which contribute to linear order in the triplet density n_t . The boxes represent the scattering amplitude Γ from Fig.1(a). The wavy line stands for the two-particle interaction μ , Eq.(4). Lines with a single arrow represent normal Green's functions (Eq.(11)) while lines with oppositely pointing arrows represent anomalous Green's functions (Eq.(12)).

FIG. 3. The coupled set of Dyson's equations for the normal and anomalous Green's functions. The anomalous self-energy (Fig.2(a)) is denoted by A . The thin lines represent the bare Green's functions, Eq.(11) (single arrow) and Eq.(12) (double arrows).

FIG. 4. The one-particle (triplet) excitation spectrum of the ladder for $J_\perp = 2J$. The solid dots represent numerical results obtained by dimer series expansions⁶ for $J_2 = 0$. The solid and dashed line are the results of the self-consistent numerical evaluation of the spectrum Eq.(21) for $J_2 = 0$ and $0.4J$, respectively. The dotted line is the $J_2 = 0$ result when only the Brueckner self-energy Eq.(13) is taken into account.

FIG. 5. One-particle spectra for $J_\perp = J$. The solid dots, open circles and solid squares are the dimer series expansion results of Ref.[13] for $J_2 = 0, 0.4J$ and $0.6J$, respectively. The solid and dashed line are the results of the self-consistent numerical evaluation of the spectrum Eq.(21) for $J_2 = 0$ and $0.4J$, respectively.

FIG. 6. (a) The bare (Born) scattering amplitude M . (b) the Bethe-Salpeter equation for the poles of the exact scattering amplitude \tilde{M} .

FIG. 7. The excitation spectrum for $J_\perp = 2J, J_2 = 0$ including the singlet bound state (long dashed line) and the triplet bound state (dot-dashed line). The solid line E_k^c is the lower edge of the two-particle continuum.

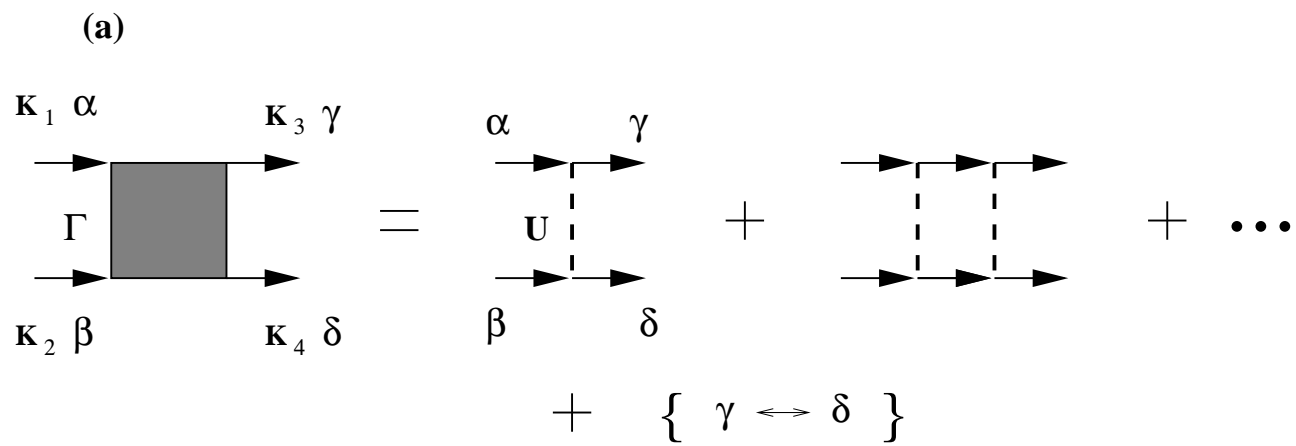
FIG. 8. Spectral function $A(k, \omega)$ for $k = 0, J_{\perp} = 2J$ and several values of J_2 obtained by Lanczos diagonalization of a 2×10 ladder. δ -functions are replaced by Lorentzians of width $0.1J$.

FIG. 9. Same as Fig.8 for $k = 0, J_{\perp} = J$.

FIG. 10. Same as Fig.9 for $k = \pi, J_{\perp} = J$.

FIG. 11. Phase diagram of the frustrated ladder from Ref.[13]. The crosses represent the line $J_2 = J$ where the ground state is a product of rung singlets.

FIG. 12. Schematic excitation spectrum on the line $J_2 = J$.



(b)

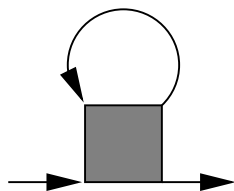


FIG.1.



FIG.2.

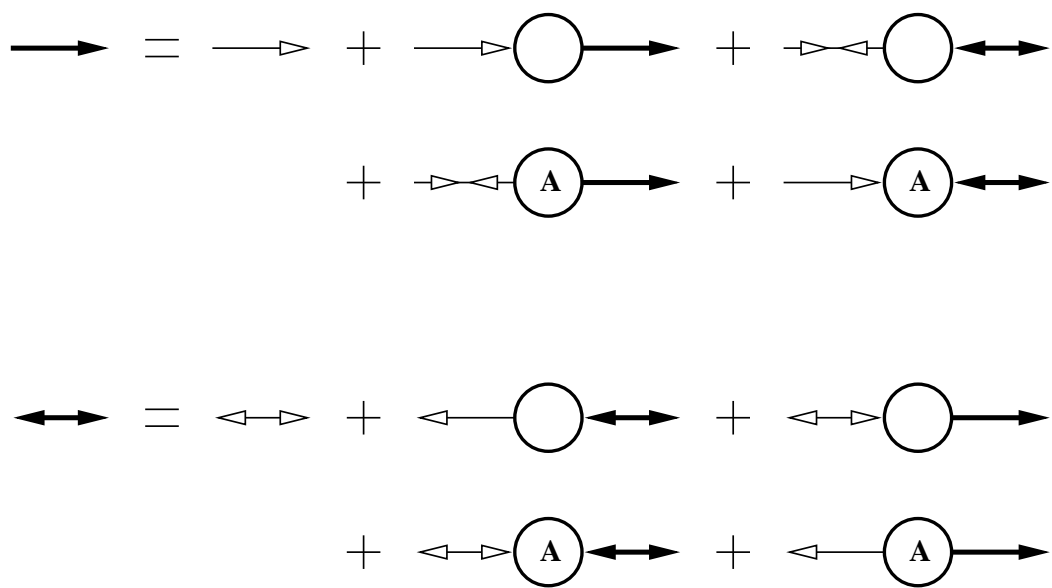


FIG.3.

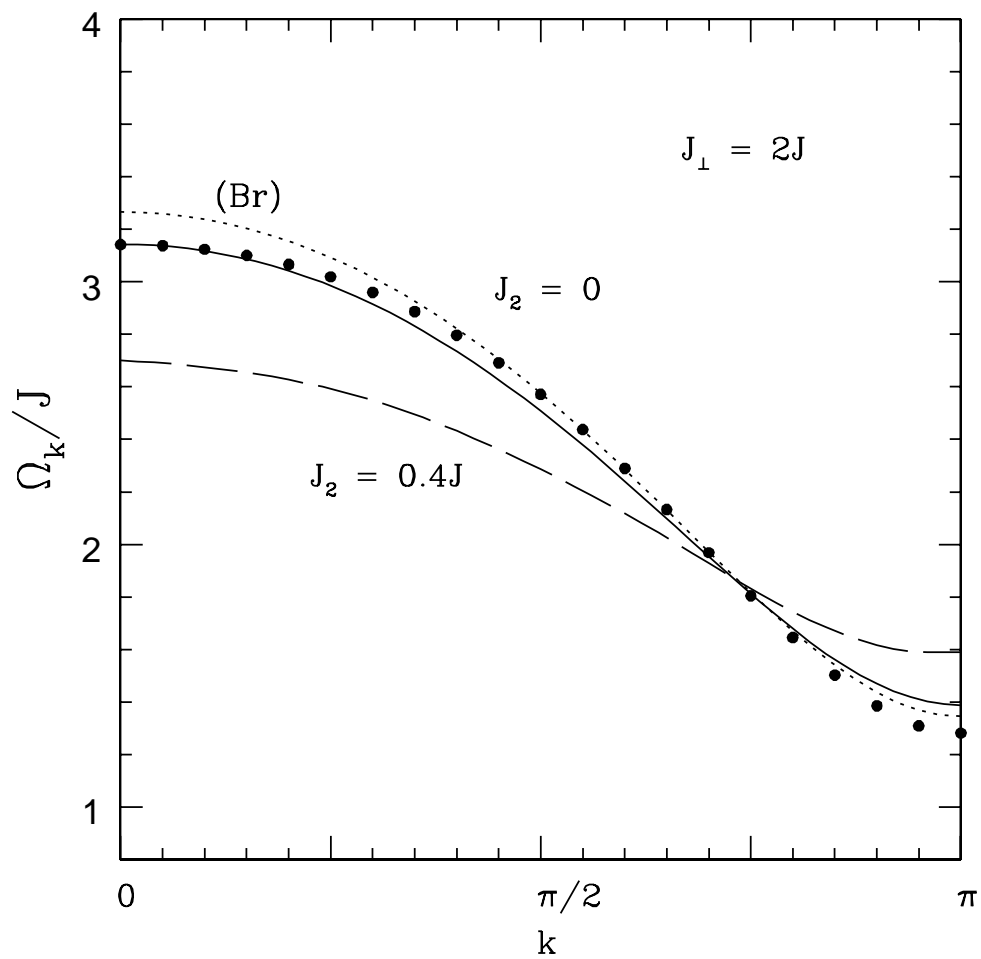


FIG.4.

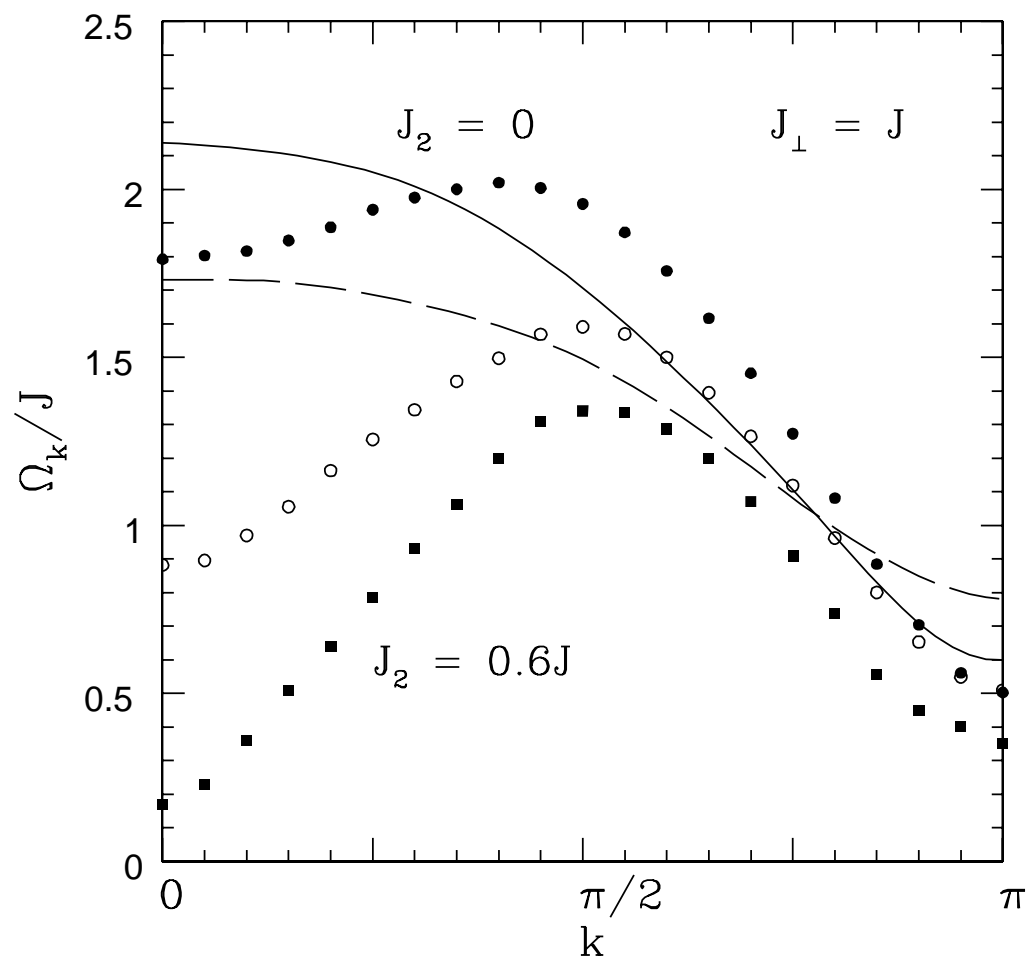
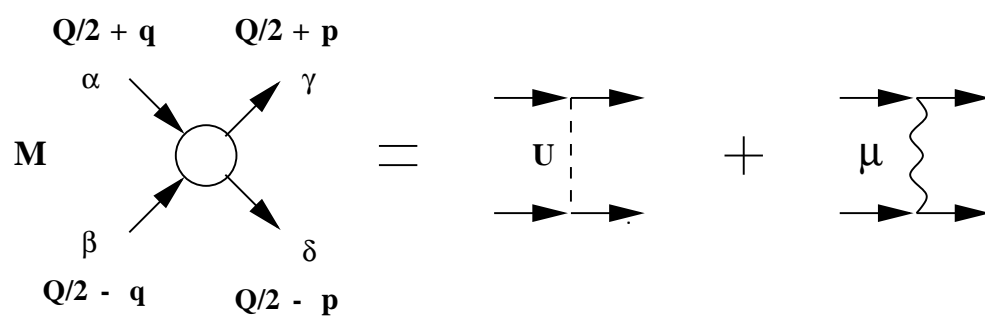


FIG.5.

(a)



(b)

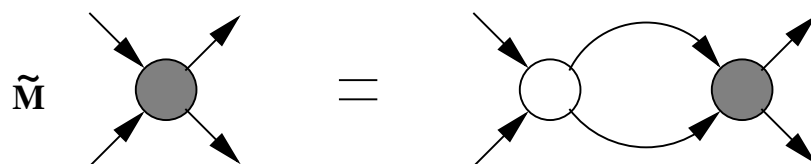


FIG.6.

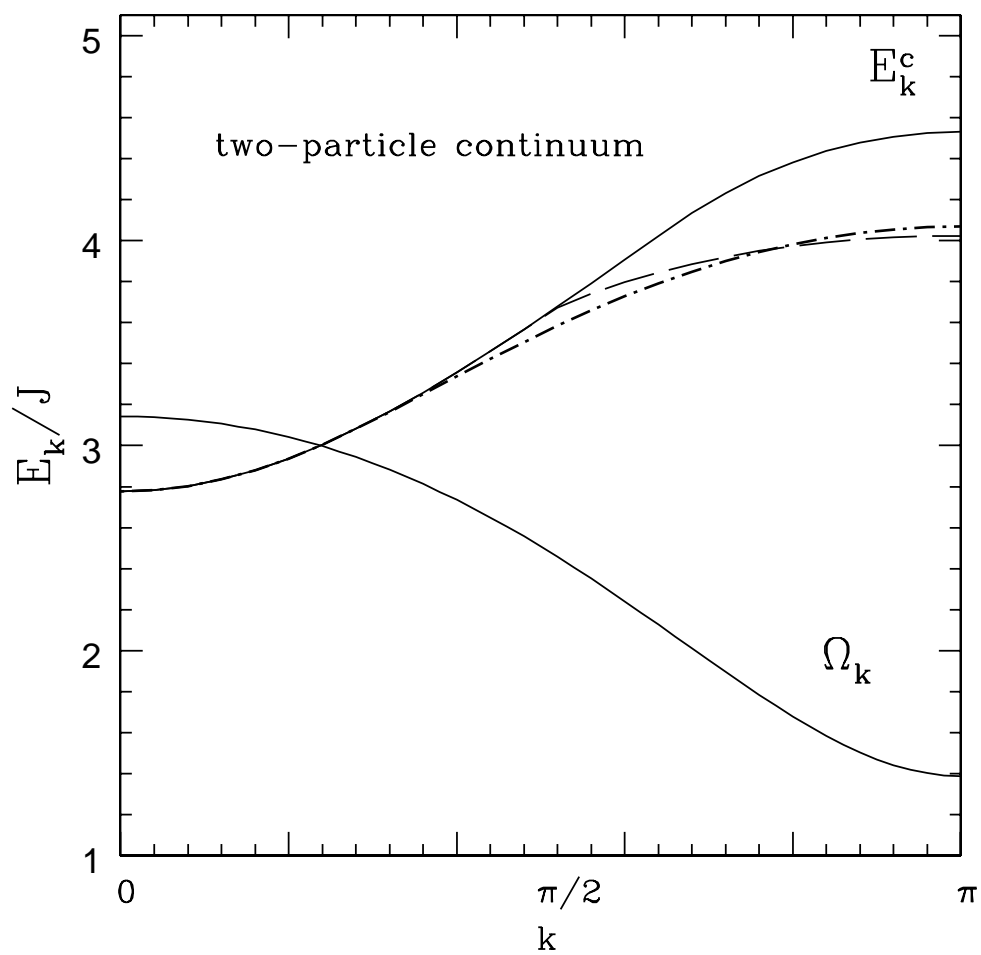


FIG.7.

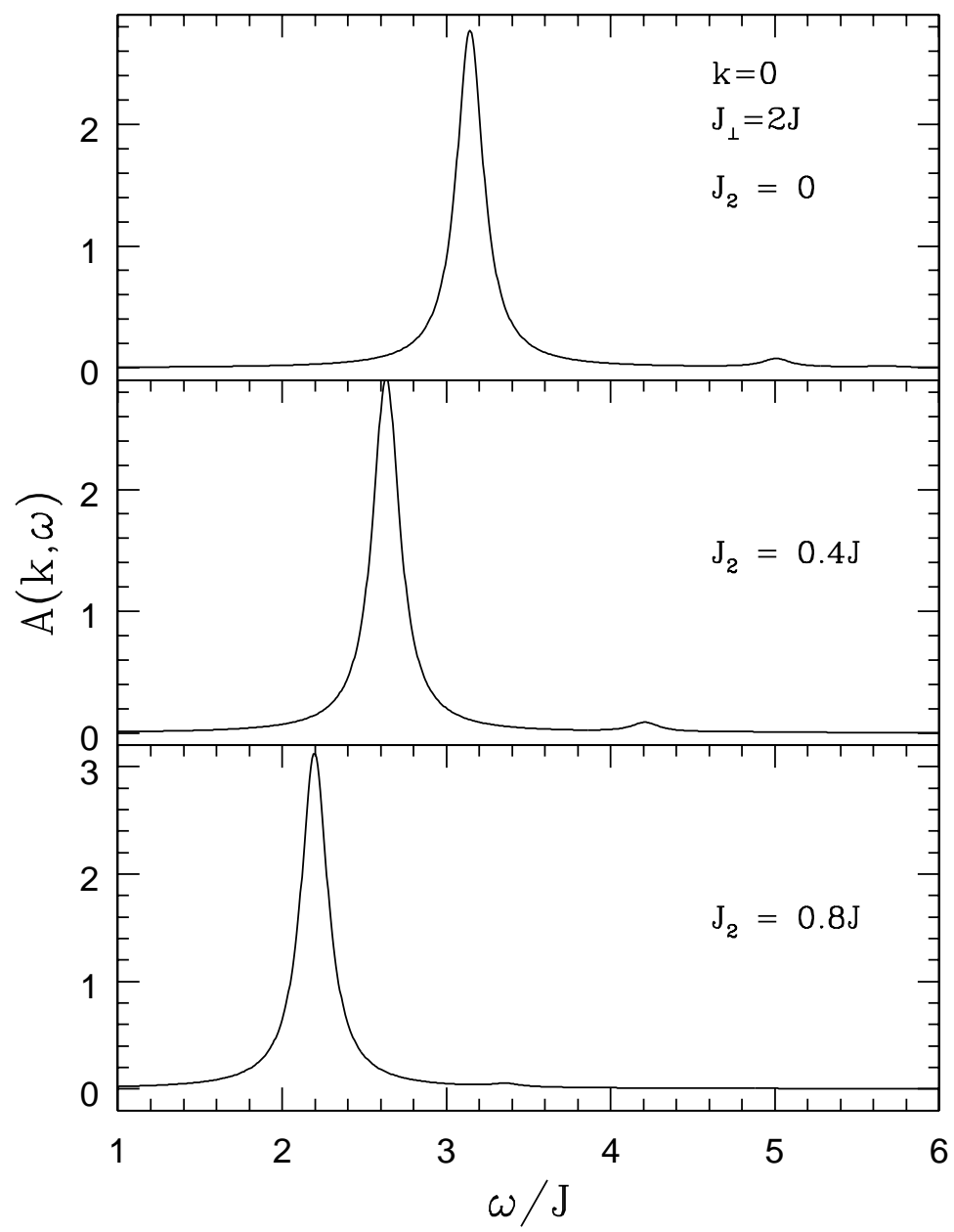


FIG.8.

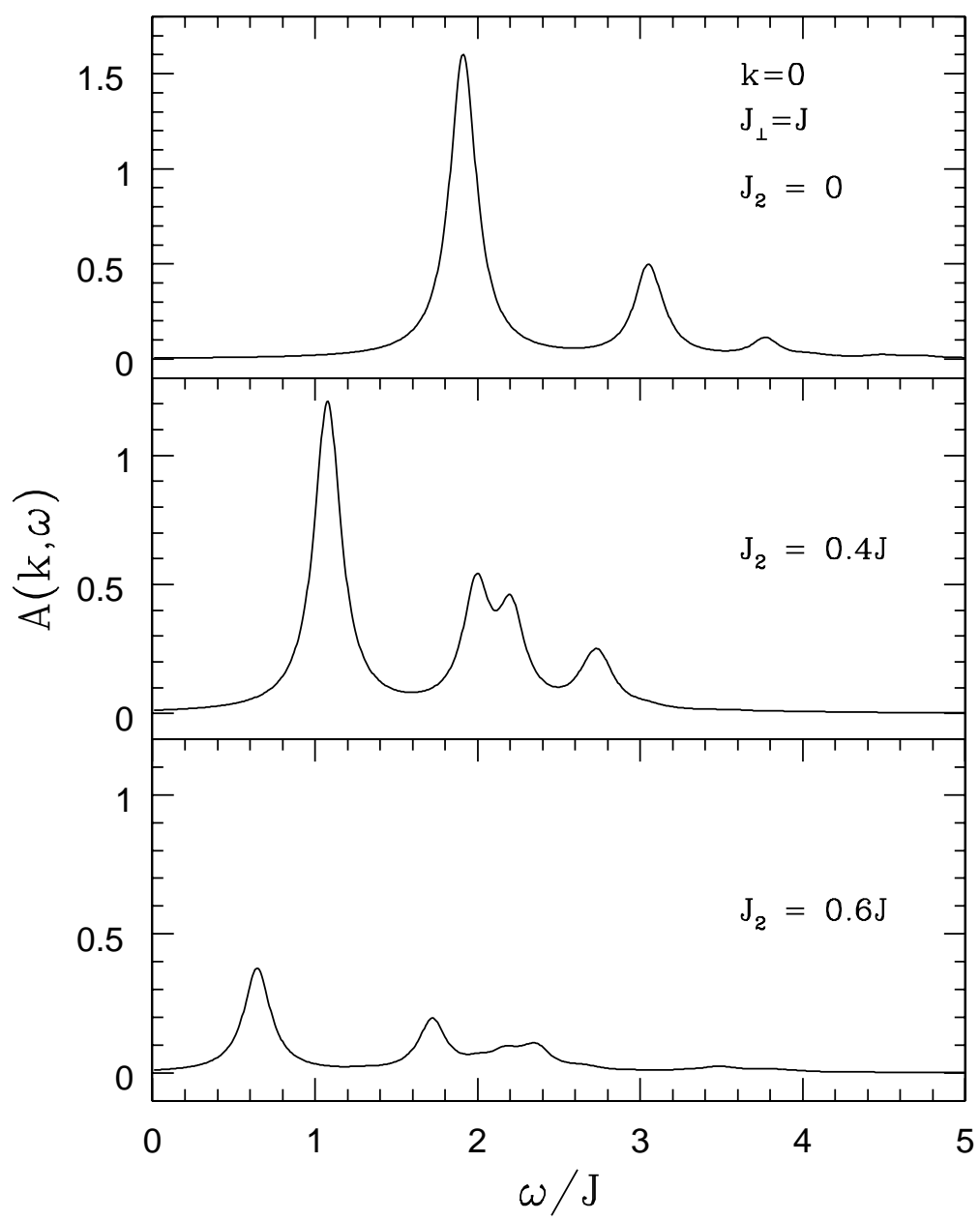


FIG.9.

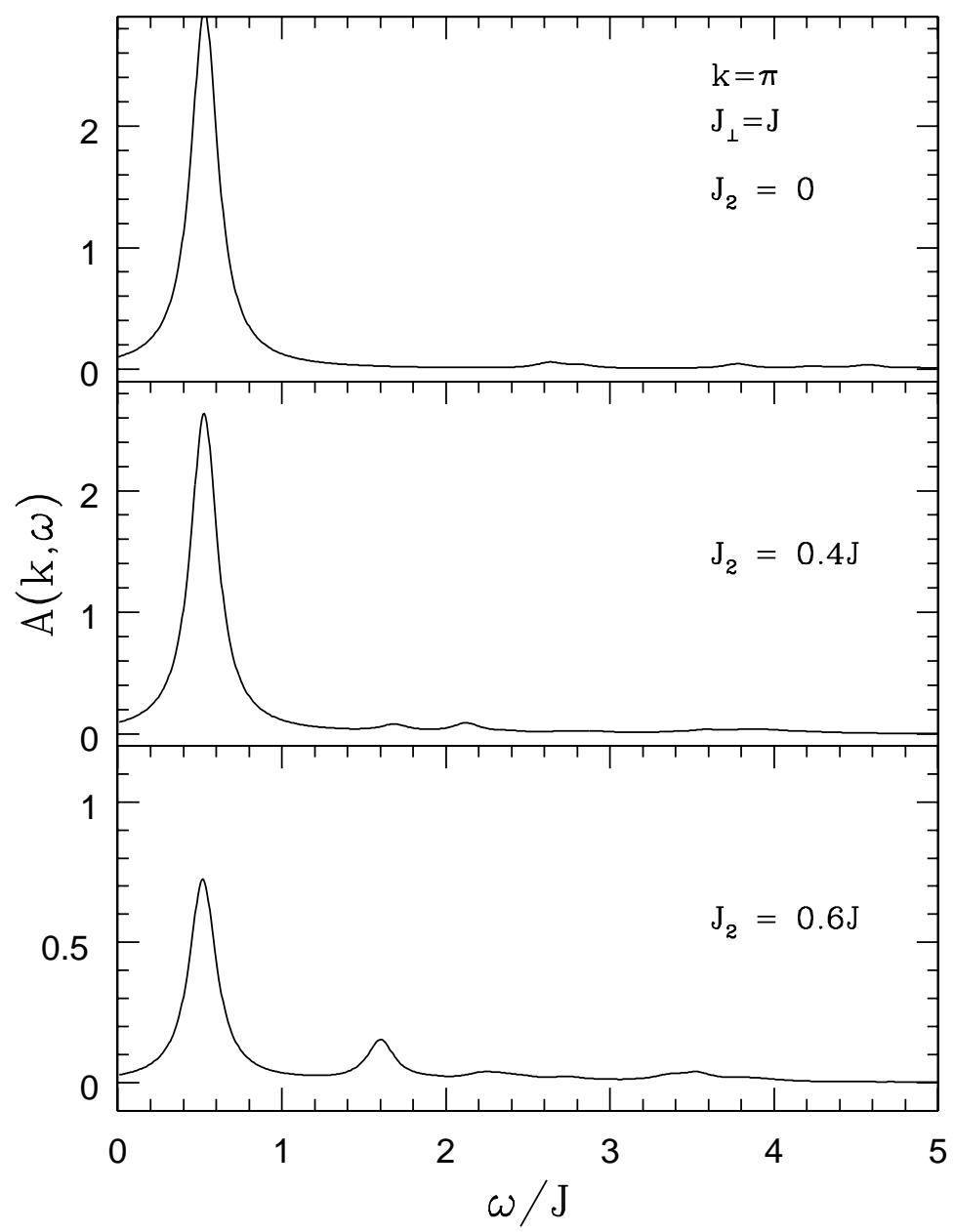


FIG.10.

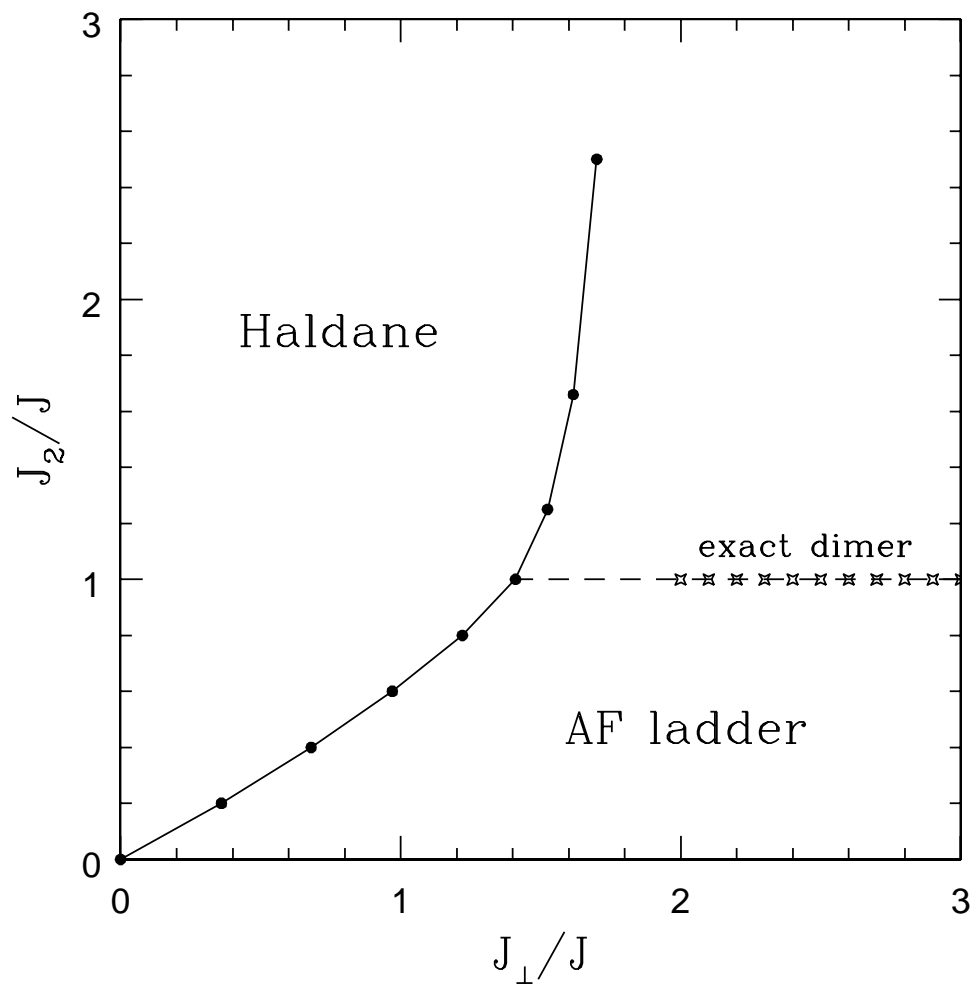


FIG.11.

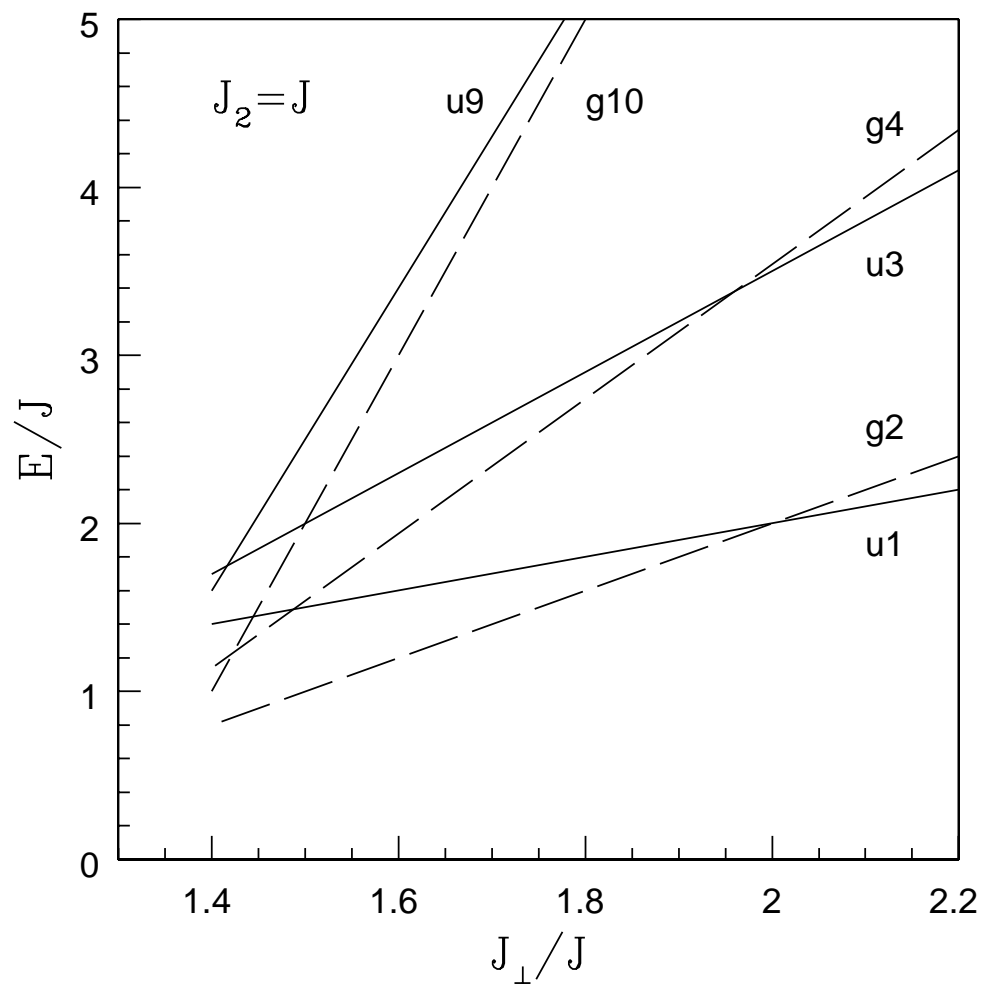


FIG.12.